Session: **Session 10: Tungsten, tungsten alloys, and advanced steels and Neutron effects in plasma-facing materials**

I-20

Molecular Dynamics Modeling and Experimental Assessment of Helium Bubble Growth, Surface Morphology Evolution, and Displacement Damage Effects in Multi-Component Alloys

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Tungsten is currently a leading candidate material for the divertor component of future fusion reactors due to it's favorable properties including high melting temperature, good thermal conductivity, and low sputtering yield. Despite these favorable properties, tungsten suffers from a high ductile-to-brittle transition temperature and a low recrystallization temperature. In addition, tungsten is also prone to microstructural damage from plasma exposure such as helium bubble and fuzz formation. This limits the use of pure tungsten as a plasma-facing material. However, alloying tungsten with other refractory metals is one way to alleviate these issues. Adding elements like Re, Ta, Ti, etc. have been shown to improve the mechanical properties of tungsten. In particular, high entropy alloys (HEAs) have shown promising properties like improved radiation tolerance. However, the role between composition and material properties is not well understood.
This talk will focus on how chemical composition affects the response of multi-component alloys (including varying amounts of W, Nb, Ta, Mo, Ti, Cr) to a fusion-relevant environment. MD simulations, using machine learning interatomic potentials, were used to identify compositions that improve the resiliency of these materials to plasma exposure and displacement damage. We simulated a range of compositions where different elements were systematically enriched or depleted over a range of 5 and 50 at%. Based on this work, we found Mo and W both served to reduce helium bubble size, whereas incorporation of Ta and W provided better resistance to displacement damage. Materials with optimized compositions were fabricated and exposed to high-flux He plasmas in the PISCES-A device at UCSD. Postmortem scanning transmission electron microscopy (STEM) and energy dispersive x-ray spectroscopy (EDS) of He-induced nanotendrils revealed that non-uniform compositional regions within the material. Compositions consistent with enhanced He bubble growth matched predictions from the MD modelling. In addition, complimentary experimental work involving exposure of specimens to divertor plasmas at DIII-D were recently completed. Post-mortem characterization and modelling of these materials is underway and will emphasize surface morphology evolution and preferential sputtering.

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